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Non-Hermitian Hamiltonians and similarity transformations

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Abstract We show that similarity (or equivalent) transformations enable one to construct non-Hermitian operators with real spectrum. In this way we can also prove and generalize the results obtained by other authors by means of a gauge-like transformation and its generalization. Such similarity transformations also reveal the connection with pseudo-Hermiticity in a simple and straightforward way. In addition to it we consider the positive and negative eigenvalues of a three-parameter non-Hermitian oscillator.

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1 Introduction

In the last years there has been great interest in the mathematical properties of non-Hermitian Hamiltonians, which was mainly aroused by the conjecture that the non-Hermitian Hamiltonians with real spectra studied so far [1–3] exhibited PT symmetry [4]. There is a vast literature on non-Hermitian Hamiltonians, some of which is reviewed elsewhere [5]. Later Mostafazadeh [6–8] showed that every Hamiltonian with a real spectrum is pseudo-Hermitian and that all the PT-symmetric Hamiltonians studied in the literature exhibited such property. On the other hand,

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the so-called space-time symmetry did not prove to be so robust in producing non-Hermitian operators with real spectra [9–12].

Some time ago Ahmed [13] derived a family of one-dimensional non-Hermitian Hamiltonians with real spectrum by means of a *gauge-like* transformation. He argued that the eigenfunctions of the resulting PT-symmetric Hamiltonian did not satisfy the PT-orthogonality condition. Recently, Rath and Mallick [14] put forward a generalization of the gauge-like transformation that involves both the coordinate and momentum operators and leads to a non-Hermitian Hamiltonian that appears to be isospectral with the harmonic oscillator.

The purpose of this paper is to discuss the gauge-like transformation in a more general and rigorous setting. In Section 2 we outline the main ideas of the similarity (or equivalent) transformation between a non-Hermitian and a Hermitian Hamiltonian. In Section 3 we discuss the gauge-like transformation introduced by Ahmed and in Section 4 the somewhat more general transformation proposed by Rath and Mallick. In Section 5 we show how to generalize the latter. In Section6 we discuss a somewhat more general three-parameter non-Hermitian oscillator and obtain its eigenvalues and eigenvectors in a somewhat different way. Finally, in Section 7 we summarize the main results and draw conclusions.

2 Similarity or equivalent transformation

Let H be a Hermitian operator with a discrete spectrum

$$H\psi_n = E_n\psi_n, \tag{1}$$

and a complete set of eigenvectors

$$\sum_n |\psi_n\rangle \langle\psi_n| = I,\ \langle\psi_m |\psi_n\rangle = \delta_{mn}, \tag{2}$$

where I is the identity operator. Its spectral decomposition reads

$$H = \sum_n E_n |\psi_n\rangle \langle\psi_n| \,. \tag{3}$$

For every linear invertible operator U the similarity transformation

$$\tilde{H} = UHU^{-1}, \tag{4}$$

yields a new operator $\tilde{H}$ that is not Hermitian unless $U^{-1} = U^{\dagger}$. We say that H and $\tilde{H}$ are equivalent or similar. The transformed vectors

$$|\varphi_n\rangle = U\,|\psi_n\rangle\,, \tag{5}$$

are eigenvectors of $\tilde{H}$

$$\tilde{H}\,|\varphi_n\rangle = UHU^{-1}U\,|\psi_n\rangle = E_n\,|\varphi_n\rangle\,, \tag{6}$$

whereas

$$|\Phi_n\rangle = \left(U^{-1}\right)^{\dagger}|\psi_n\rangle\,, \tag{7}$$

are eigenvectors of the adjoint operator $\tilde{H}^{\dagger}$

$$\tilde{H}^{\dagger}\,|\Phi_n\rangle = \left(U^{-1}\right)^{\dagger}HU^{\dagger}\left(U^{-1}\right)^{\dagger}|\psi_n\rangle = E_n\,|\Phi_n\rangle\,. \tag{8}$$

Both sets of vectors form a biorthonormal basis

$$\langle\Phi_m\,|\varphi_n\rangle = \langle\psi_m\,|\psi_n\rangle = \delta_{mn}, \tag{9}$$

that enables us to write

$$\tilde{H} = \sum_n E_n U\,|\psi_n\rangle\,\langle\psi_n|\,U^{-1} = \sum_n E_n\,|\varphi_n\rangle\,\langle\Phi_n|\,. \tag{10}$$

The basis set $\{|\varphi_n\rangle\}$ is orthonormal with the metric given by $\left(U^{-1}\right)^{\dagger}U^{-1}$:

$$\langle\psi_m\,|\psi_n\rangle = \langle\varphi_m|\left(U^{-1}\right)^{\dagger}U^{-1}\,|\varphi_n\rangle = \delta_{mn}. \tag{11}$$

On the other hand, the standard inner product

$$\langle\varphi_m\,|\varphi_n\rangle = \langle\psi_m|\,U^{\dagger}U\,|\psi_n\rangle\,, \tag{12}$$

is not necessarily finite.

It follows from (4) that

$$\tilde{H}^{\dagger} = \left(U^{-1}\right)^{\dagger}HU^{\dagger} = \left(U^{-1}\right)^{\dagger}U^{-1}\tilde{H}UU^{\dagger} = \eta\tilde{H}\eta^{-1} \tag{13}$$

where $\eta = \left(U^{-1}\right)^{\dagger}U^{-1}$ is Hermitian and positive definite. We say that $\tilde{H}$ is η-pseudo-Hermitian [6–8] and (11) becomes

$$\langle\varphi_m|\,\eta\,|\varphi_n\rangle = \delta_{mn}. \tag{14}$$

If A and B are two linear operators then

$$[\tilde{A}, \tilde{B}] = U[A, B]U^{-1}. \tag{15}$$

In particular, the commutator $[x, p] = iI$ between the coordinate x and momentum p is conserved

$$[\tilde{x}, \tilde{p}] = iI. \tag{16}$$

Summarizing: a non-Hermitian operator $\tilde{H}$ that is similar or equivalent to an Hermitian one H is pseudo Hermitian. In addition to it, both operators are isospectral. When the similarity transformation is unitary ($U^{-1} = U^{\dagger}$) it conserves the norm ($\langle \varphi_m \mid \varphi_n \rangle = \delta_{mn}$), $\eta = I$ and $\tilde{H}$ is obviously Hermitian.

The results developed above are not new since they are contained in Mostafazadeh's papers [6–8]. We simply derived them here from the point of view of a similarity transformation in order to connect them with the papers of Ahmed [13] and Rath and Mallick [14] in a clearer way.

3 Gauge-like transformation

The gauge-like transformation for one-dimensional operators

$$H = \frac{1}{2}p^2 + V(x), \tag{17}$$

discussed by Ahmed [13] is a particular case of the similarity transformation outlined in Section 2. If we choose

$$U = e^{u(x)}, \tag{18}$$

then [15]

$$\tilde{p} = UpU^{-1} = p + [u, p] = p + iu', \ \tilde{x} = x, \tag{19}$$

and

$$\tilde{H} = \frac{1}{2}(p + iu')^2 + V(x). \tag{20}$$

Therefore, H and $\tilde{H}$ are isospectral as discussed in Section 2.

The transformation of the non-Hermitian operator

$$H_\beta = \frac{1}{2}[p + i\beta\nu(x)]^2 + V(x), \tag{21}$$

yields

$$\tilde{H}_\beta = \frac{1}{2}[p + i\beta\nu(x) + iu'(x)]^2 + V(x). \tag{22}$$

If $\nu(x)$ is real and

$$u'(x) = -2\beta\nu(x), \tag{23}$$

then

$$\tilde{H}_\beta = H_\beta^\dagger. \tag{24}$$

Since $u(x)$ is real then U is Hermitian and positive definite; therefore H_β is U-pseudo-Hermitian.

In particular, Ahmed chose $\nu(x) = x$ and $V(x) = \left(\alpha^2 + \beta^2\right) x^2/2$ so that

$$H_\beta = \frac{1}{2}(p + i\beta x)^2 + \frac{1}{2}\left(\alpha^2 + \beta^2\right) x^2, \tag{25}$$

and $u(x) = u_1(x) = -\beta x^2$ leads to equation (24). Note that if $u_2(x) = -\beta x^2/2$ then

$$e^{u_2} H_\beta e^{-u_2} = \frac{1}{2}p^2 + \frac{1}{2}\left(\alpha^2 + \beta^2\right) x^2 = H_{SHO} \tag{26}$$

from which we conclude that H_β and the simple harmonic oscillator H_{SHO} are isospectral. In this case the eigenfunctions $\varphi_n(x)$ of the former operator are square integrable provided $\alpha \neq 0$ [13]. These results are particular cases of those derived in Section 2 (note that $e^{u_2}\left(e^{u_2}\right)^\dagger = e^{u_1}$).

Ahmed [13] also discussed the particular case $\beta = i\gamma$, γ real, that leads to the Hermitian operator

$$H_\gamma = \frac{1}{2}(p - \gamma x)^2 + \frac{1}{2}\left(\alpha^2 - \gamma^2\right) x^2, \tag{27}$$

and draw two curious conclusions. He stated that "Remarkably, the usual connection between the nodal structure with the quantum number n does not hold any more. Even the ground state may have nodes for some values of γ." Since $|\varphi_n(x)| = |\psi_n(x)|$ it is obvious that both functions have the same number of nodes; in particular, the ground state $\varphi_0(x)$ is nodeless in the interval $(-\infty, \infty)$ as expected. He also said that "Eigenvalues (18) possess an interesting feature of becoming complex (conjugate) at the cost of eigenfunction (19) being delocalized as it would not vanish at $x = \pm\infty$. This interesting phase-transition of eigenvalues from real to complex takes place when $\gamma > \gamma_{critical}$ $(= \alpha)$." It is obvious that this *interesting phase transition* is due to the force constant chosen for H_{SHO} and has

nothing to do with the transformation of one oscillator into the other. To see this point more clearly just choose

$$H_\gamma = \frac{1}{2}(p-\gamma x)^2 + \frac{1}{2}kx^2, \tag{28}$$

and the phase transition does not take place for any value of γ if $k > 0$.

4 Transformation of coordinate and momentum

Recently, Rath and Mallick [14] proposed the following generalization of the gauge-like transformation:

$$x \rightarrow \tilde{x} = \frac{1}{\sqrt{1+\alpha\beta}}\left(x + i\alpha p\right),\; p \rightarrow \tilde{p} = \frac{1}{\sqrt{1+\alpha\beta}}\left(p + i\beta x\right), \tag{29}$$

that converts

$$H_{HO} = \frac{1}{2}\left(p^2 + x^2\right) \tag{30}$$

into the non-Hermitian operator

$$H = \frac{1}{2(1+\alpha\beta)}\left[(p+i\beta x)^2 + (x+i\alpha p)^2\right]. \tag{31}$$

By means of a non-rigorous procedure based on second quantization, an adjustable frequency and a truncated perturbation expansion they conjectured that the eigenvalues of H appeared to be exactly those of H_{HO}.

This conclusion follows straightforwardly from the similarity transformation

$$H = UH_{HO}U^{-1}, \tag{32}$$

where U is given by

$$UxU^{-1} = \tilde{x},\; UpU^{-1} = \tilde{p} \tag{33}$$

According to the results of Section 2 both operators are isospectral with eigenvalues

$$E_n = n + \frac{1}{2},\; n = 0, 1, \ldots, \tag{34}$$

and H is η-pseudo-Hermitian.

It only remains to determine whether the eigenfunctions of H are square integrable. To this end we resort to the construction of the eigenvectors of H_{HO} in second-quantization form [15]:

$$a\left|\psi_0\right\rangle = 0,\; \left|\psi_n\right\rangle = \frac{1}{\sqrt{n!}}\left(a^\dagger\right)^n\left|\psi_0\right\rangle, \tag{35}$$

where

$$a=\frac{1}{\sqrt{2}}\left(x+ip\right),\ a^{\dagger}=\frac{1}{\sqrt{2}}\left(x-ip\right). \tag{36}$$

It follows from equations (29), (33) and (35) that

$$\tilde{a}\left|\varphi_0\right\rangle=0,\ \left|\varphi_n\right\rangle=\frac{1}{\sqrt{n!}}\left(\tilde{a}^{\dagger}\right)^n\left|\varphi_0\right\rangle. \tag{37}$$

Since

$$\tilde{a}=\frac{1}{\sqrt{2(1+\alpha\beta)}}\left[(1-\beta)x+i(1+\alpha)p\right], \tag{38}$$

then the ground state $\varphi_0(x)$ is a solution of the first-order differential equation

$$\varphi_0'(x)=-\frac{1-\beta}{1+\alpha}\varphi_0(x), \tag{39}$$

that leads to

$$\varphi_0(x)=\left[\frac{1-\beta}{\pi(1+\alpha)}\right]^{1/4}\exp\left[-\frac{1-\beta}{2(1+\alpha)}x^2\right]. \tag{40}$$

We appreciate that $\varphi_0(x)$ is square integrable (and, consequently, also all the other eigenfunctions $\varphi_n(x)$) provided that $\beta<1$ and $\alpha>-1$. The square-integrability of the eigenfunctions was not discussed by Rath and Mallick [14] in spite of the fact that the conditions just given appear explicitly in the zero and pole of their chosen frequency ω for Case II.

The operator that carries out the transformation (29) is of the form [15]

$$U=\exp\left(ax^2+bp^2\right), \tag{41}$$

where

$$\begin{aligned} i\alpha &= \frac{\left(e^{2\sqrt{-ab}}-1\right)\sqrt{-ab}}{a\left(e^{2\sqrt{-ab}}+1\right)} \\ i\beta &= \frac{\left(1-e^{2\sqrt{-ab}}\right)\sqrt{-ab}}{b\left(e^{2\sqrt{-ab}}+1\right)}, \end{aligned} \tag{42}$$

that leads to $\alpha/\beta=-b/a$.

5 A more general coordinate-momentum transformation

A more general similarity transformation is given by [15]

$$\begin{aligned}\tilde{x} &= UxU^{-1} = U_{11}x + U_{12}p \\ \tilde{p} &= UpU^{-1} = U_{21}x + U_{22}p,\end{aligned} \tag{43}$$

where

$$U_{11}U_{22} - U_{21}U_{12} = 1, \tag{44}$$

follows from the condition $[\tilde{x}, \tilde{p}] = iI$. Since the matrix elements U_{ij} may be complex numbers the transformation depends on 8 parameters that should satisfy two equations; therefore, there are only 6 independent parameters and the transformation is given by an exponential operator of the form [15]

$$U = \exp\left[\frac{a}{2}x^2 + \frac{c}{2}(xp + px) + \frac{b}{2}p^2\right], \tag{45}$$

where a, b and c are complex numbers.

The application of this similarity transformation to the harmonic oscillator H_{HO} (30) yields the operator

$$\begin{aligned}\tilde{H} &= UH_{HO}U^{-1} \\ &= \frac{1}{2}\left[\left(U_{22}^2 + U_{12}^2\right)p^2 + \left(U_{11}^2 + U_{21}^2\right)x^2 + \left(U_{21}U_{22} + U_{11}U_{12}\right)(xp + px)\right].\end{aligned} \tag{46}$$

By means of well known operator formulas [15] it is not difficult to prove that

$$\begin{aligned}U_{11} &= \cosh(\theta) - \frac{c}{\theta}\sinh(\theta) \\ U_{12} &= -\frac{b}{\theta}\sinh(\theta) \\ U_{21} &= \frac{a}{\theta}\sinh(\theta) \\ U_{22} &= \cosh(\theta) + \frac{c}{\theta}\sinh(\theta) \\ \theta &= \sqrt{c^2 - ab}\,.\end{aligned} \tag{47}$$

In general, any operator of the form (46) with matrix elements U_{ij} that satisfy the condition (44) is equivalent (and therefore isospectral) to the harmonic oscillator (30). It is always η-pseudo-Hermitian and under certain conditions it may also be Hermitian or PT-symmetric. For example, if $U_{22}^2 + U_{12}^2$ and $U_{11}^2 + U_{21}^2$ are both real

and $(U_{21}U_{22}+U_{11}U_{12})$ purely imaginary, then $\tilde{H}$ is PT-symmetric. The choice $U_{11}=U_{22}=1$, $U_{12}=0$, and $U_{21}=i\beta$ yields one of the examples given by Ahmed [13]. On he other hand, when $U_{11}=U_{22}=1/\sqrt{1+\alpha\beta}$, $U_{12}=i\alpha/\sqrt{1+\alpha\beta}$, and $U_{21}=i\beta/\sqrt{1+\alpha\beta}$ we obtain the model proposed by Rath and Mallick [14]. Obviously, when the coefficients of p^2, x^2 and $xp+px$ are real $\tilde{H}$ is Hermitian.

Arguing as in Section 4 we conclude that the eigenfunctions $\varphi_n(x)$ of $\tilde{H}$ are square integrable provided that

$$\Re\frac{U_{11}+iU_{21}}{U_{22}-iU_{12}}>0 \tag{48}$$

6 Positive and negative eigenvalues

By a suitable choice of the adjustable frequency Rath [16] managed to obtain negative harmonic-oscillator-like eigenvalues. However, the author did not consider the square integrability of the eigenfunctions with sufficient detail. In order to analyze this aspect of the problem we resort to a different approach.

Consider the non-Hermitian Hamiltonian

$$H=h_{11}p^2+ih_{12}(xp+px)+h_{22}x^2, \tag{49}$$

where $[x,p]=i$ and the coefficients h_{ij} are real. In order to obtain its spectrum we express the coordinate and momentum operators in terms of the creation $a^\dagger$ and annihilation a operators as

$$x=\frac{1}{\sqrt{2\omega}}\left(a+a^\dagger\right),\ p=i\sqrt{\frac{\omega}{2}}\left(a^\dagger-a\right), \tag{50}$$

where $[a,a^\dagger]=1$. The Hamiltonian operator (49) then becomes

$$\begin{aligned}H=&\left(\frac{h_{11}\omega}{2}+\frac{h_{22}}{2\omega}\right)\left(2a^\dagger a+1\right)\\&+\left(-\frac{h_{11}\omega}{2}+h_{12}+\frac{h_{22}}{2\omega}\right)a^2\\&+\left(-\frac{h_{11}\omega}{2}-h_{12}+\frac{h_{22}}{2\omega}\right)\left(a^\dagger\right)^2.\end{aligned} \tag{51}$$

We expand every eigenvector $|\psi\rangle$ of H in the basis set of eigenvectors $\{|n\rangle\,,\ n=0,1,\ldots\}$ of the occupation number operator $a^\dagger a$

$$|\psi\rangle=\sum_{n=0}^{\infty}d_n\,|n\rangle \tag{52}$$

that satisfy

$$a\left|n\right\rangle=\sqrt{n}\left|n-1\right\rangle,\;a^{\dagger}\left|n\right\rangle=\sqrt{n+1}\left|n+1\right\rangle. \tag{53}$$

It follows from (51) and (53) that

$$H\left|n\right\rangle=A_{n}(\omega)\left|n-2\right\rangle+B_{n}(\omega)\left|n\right\rangle+C_{n}(\omega)\left|n+2\right\rangle, \tag{54}$$

where

$$\begin{aligned} A_{n}(\omega) &= \left(-\frac{h_{11}\omega}{2}+h_{12}+\frac{h_{22}}{2\omega}\right)\sqrt{n(n-1)} \\ B_{n}(\omega) &= \left(\frac{h_{11}\omega}{2}+\frac{h_{22}}{2\omega}\right)(2n+1) \\ C_{n}(\omega) &= \left(-\frac{h_{11}\omega}{2}-h_{12}+\frac{h_{22}}{2\omega}\right)\sqrt{(n+1)(n+2)}. \end{aligned} \tag{55}$$

It follows from $H\left|\psi\right\rangle=E\left|\psi\right\rangle$ and equation (54) that

$$A_{n+2}d_{n+2}+(B_{n}-E)\,d_{n}+C_{n-2}d_{n-2}=0. \tag{56}$$

Note that $C_{n}(\omega)=0$ for all n if

$$\omega=\begin{cases}\omega_{+}=\frac{\sqrt{h_{11}h_{22}+h_{12}^{2}}-h_{12}}{h_{11}}>0\\ \omega_{-}=-\frac{\sqrt{h_{11}h_{22}+h_{12}^{2}}+h_{12}}{h_{11}}<0\end{cases}. \tag{57}$$

For either of these values of ω we have

$$d_{n+2}=\frac{E-B_{n}}{A_{n+2}}d_{n}, \tag{58}$$

so that

$$\left|\psi_{k,s}\right\rangle=\sum_{j=0}^{k}d_{2j+s}\left|2j+s\right\rangle,\;E_{k,s}=B_{2k+s}, \tag{59}$$

where $k=0,1,\ldots$ and $s=0$ or $s=1$ give us the even or odd states, respectively. It is worth noting that the eigenvectors of H are not exactly those of the occupation number operator, except when $k=0$. Rath [16], on the other hand, appears to suggest that both H and $a^{\dagger}a$ have a common set of eigenvectors in spite of the fact that these operators do not commute.

The ground state eigenfunction $\psi_{0}(x)=\left\langle x\right|\left.\psi_{0}\right\rangle$ obtained from $\left\langle x\right|a\left|\psi_{0}\right\rangle=0$ is square integrable when $\omega>0$ as follows from

$$\psi_{0}(x)=\frac{|\omega|^{1/4}}{\pi^{1/4}}\exp\left(-\omega x^{2}/2\right). \tag{60}$$

Therefore, for $\omega = \omega_+$ we have

$$E_n(\omega_+) = \sqrt{h_{11}h_{22} + h_{12}^2}\,(2n+1)\,, \tag{61}$$

where $n = 2k + s$ takes into account the even and odd states simultaneously. On the other hand, when $\omega = \omega_-$

$$E_n(\omega_-) = -\sqrt{h_{11}h_{22} + h_{12}^2}\,(2n+1)\,, \tag{62}$$

and the eigenfunctions $\psi_n(x) = \langle x|\,\psi_n\rangle$ are square integrable along the imaginary axis ix.

The three-parameter Hamiltonian (49) is obviously more general than the two-parameter one discussed by Rath and Malick [14] and Rath [16] where

$$h_{11} = \frac{1-\lambda^2}{2(1+\lambda\beta)},\; h_{12} = \frac{\lambda+\beta}{2(1+\lambda\beta)},\; h_{22} = \frac{1-\beta^2}{2(1+\lambda\beta)}. \tag{63}$$

Note that in this particular case $h_{11}h_{22} + h_{12}^2 = \frac{1}{4}$ and

$$\begin{aligned} \omega_1 &= \frac{1-\beta}{1+\lambda} \\ \omega_2 &= \frac{1+\beta}{\lambda-1}. \end{aligned} \tag{64}$$

7 Conclusions

The purpose of this paper is to show that the results of Ahmed [13] and Rath and Mallick [14] can be straightforwardly derived and proved by suitable similarity transformations. In the former case there is no need of discussing the reality of the operator and its eigenfunctions or the orthogonality conditions. In fact, the proposition enunciated by the author does not explain the situation. Once we prove that a non-Hermitian operator is similar to an Hermitian one the reality of the spectrum of the former is certainly proved. Of course, caution must be exercised with respect to the square-integrability of its eigenfunctions.

With respect to the latter paper [14] the similarity transformation is a much more rigorous and straightforward way of proving that the non-Hermitian operator is isospectral with the harmonic oscillator. The results of both papers are merely particular cases of the general expressions derived by Mostafazadeh [6–8] and also of the equations derived in Section 2.

Equation (46) with the restriction (44) enables us to construct a family of non-Hermitian operators with real spectrum. If necessary we can enlarge the number of cases by choosing $H_{HO} = p^2 + kx^2$, $k > 0$, instead of the operator (30) thus having one more independent parameter at our disposal.

We have also shown how to obtain the eigenvalues and eigenvectors of a more general three-parameter oscillator by a judicious modification of the procedure proposed by Rath and Mallick [14] and Rath [16]. Present approach is completely rigorous (unlike the perturbation approach [14]) and reveals that the eigenvectors of the non-Hermitian operator are not exactly those of the occupation number operator (as suggested by Rath [16]) but linear combinations of them.

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